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                BEILSTEIN enhanced with new display and select options,
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                 Patent Office Classifications
                The Analysis Edition of STN Express with Discover!
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        AUG 27
        AUG 27 BIOTECHABS/BIOTECHDS: Two new display fields added for legal
NEWS
                 status data from İNPADOC
        SEP 01
                 INPADOC: New family current-awareness alert (SDI) available
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NEWS 10
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                 STN Express with Discover!
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        SEP 01
                New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
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        SEP 27
                STANDARDS will no longer be available on STN
NEWS 13
        SEP 27 SWETSCAN will no longer be available on STN
            JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT
NEWS EXPRESS
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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              STN Operating Hours Plus Help Desk Availability
              General Internet Information
NEWS INTER
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              Welcome Banner and News Items
NEWS PHONE
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Uploading

Page 1

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#### => FILE REGISTRY

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ENTRY SESSION
FULL ESTIMATED COST 0.21 0.21

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STRUCTURE FILE UPDATES: 20 OCT 2004 HIGHEST RN 766487-31-4 DICTIONARY FILE UPDATES: 20 OCT 2004 HIGHEST RN 766487-31-4

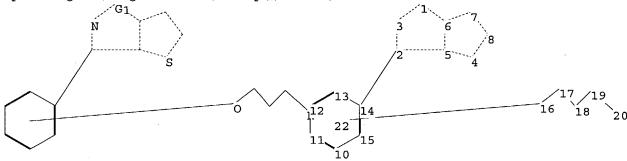
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Crossover limits have been increased. See HELP CROSSOVER for details.

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=> Uploading C:\Program Files\Stnexp\Queries\10088250.str



chain nodes :

16 17 18 19 20

ring nodes :

1 2 3 4 5 6 7 8 10 11 12 13 14 15

chain bonds :

2-14 16-17 17-18 18-19 19-20

ring bonds :

10/21/2004

10088250.trn

1-6 1-3 2-5 2-3 4-5 4-8 5-6 6-7 7-8 10-11 10-15 11-12 12-13 13-14 14-15

exact/norm bonds :

1-6 1-3 2-5 2-3 2-14 4-5 4-8 5-6 6-7 7-8 16-17 17-18 18-19 19-20

normalized bonds :

10-11 10-15 11-12 12-13 13-14 14-15

isolated ring systems :

containing 1 : 10 :

G1:0,N

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:Atom 11:Atom

12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS

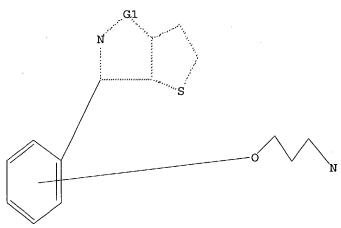
20:CLASS 22:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 0, N

Structure attributes must be viewed using STN Express query preparation.

5 ANSWERS

=> s 11

SAMPLE SEARCH INITIATED 08:54:58 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 8 TO ITERATE

100.0% PROCESSED 8 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 8 TO 329

PROJECTED ANSWERS: 5 TO 2

1.2

5 SEA SSS SAM L1

=> s l1 sss full

FULL SEARCH INITIATED 08:55:04 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 201 TO ITERATE

100.0% PROCESSED

201 ITERATIONS

SEARCH TIME: 00.00.01

T.3

131 SEA SSS FUL L1

=> FIL CAPLUS

COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE

TOTAL

ENTRY

SESSION

155.42

155.63

131 ANSWERS

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13

L4

=> d l4 ibib abs hitstr tot

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

2001:208282 CAPLUS

DOCUMENT NUMBER:

134:237472

TITLE:

Préparation of 1-amino-3-thienoisoxazolylphenoxy-2-

INVENTOR(S):

propanols as dopamine D4 antagonists
Fink, David M.; Freed, Brian S.; Hrib, Nicholas J.; Kosley, Raymond W., Jr.; Lee, George E.; Merriman,

Gregory H.; Rauckman, Barbara S. Aventis Pharmaceuticals, Inc., USA

PCT Int. Appl., 157 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

SOURCE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT ASSIGNEE(S):

Page 4

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KIND
                                 DATE
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                                                                       DATE
     PATENT NO.
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     WO 2001019833
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PRIORITY APPLN. INFO.:
                                              US 1999-396081
                                                                    A1 19990914
                                              WO 2000-US24962
                                                                      20000913
OTHER SOURCE(S):
                          MARPAT 134:237472
     RZOCH2CR1R2CH2NR3R4 [I; R = e.g., thieno[2,3-d]isoxazol-3-yl; R1 = OH or
     alkoxy; R2,R4 = H or alkyl; R3 = CH2R5, CH2CH(OH)R5, indanyl, etc.; R5 =
     cyclohex(en)yl, (hetero)aryl, etc.; Z = phenylene] were prepared Thus,
     3-bromothiophene was acylated by 3-(MeO)C6H4COCl and the oximated product
     cyclized to give, after O-demethylation, 3-RC6H4OH [R =
     thieno[2,3-d]isoxazol-3-yl] which was etherified by (R)-glycidyl tosylate
     and the product aminated by PhCHMeNH2 to give (R)-3-
     RC6H4OCH2CH(OH)CH2NMeCH2Ph (R as above). Data for biol. activity of I
     were given.
     330650-04-9P 330650-17-4P 330650-18-5P
IT
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RN

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 1-amino-3-thienoisoxazolylphenoxy-2-propanols as dopamine D4 antagonists)

330650-04-9 CAPLUS

2-Propanol, 1-[methyl(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

### ● HCl

RN 330650-17-4 CAPLUS

CN 2-Propanol, 1-[(2-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-18-5 CAPLUS

CN 2-Propanol, 1-[(1-naphthalenylmethyl)amino]-3-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-19-6 CAPLUS

CN 2-Propanol, 1-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(3-thienylmethyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-20-9 CAPLUS

CN 2-Propanol, 1-[(2-furanylmethyl)amino]-3-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-21-0 CAPLUS

CN 2-Propanol, 1-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-22-1 CAPLUS

CN 2-Propanol, 2-methyl-1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

RN 330650-23-2 CAPLUS

CN 2-Propanol, 2-methyl-1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2R)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 330650-22-1 CMF C20 H20 N2 O3 S2

Absolute stereochemistry.

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

$$HO_2C$$
 $Z$ 
 $CO_2H$ 

RN 330650-24-3 CAPLUS

CN 2-Propanol, 1-[[(4-methoxyphenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

RN 330650-25-4 CAPLUS

CN 2-Propanol, 1-[[(2-methoxyphenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-26-5 CAPLUS

CN 2-Propanol, 1-[[(4-chlorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-27-6 CAPLUS

CN 2-Propanol, 1-[[(4-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-28-7 CAPLUS

CN 2-Propanol, 1-[[(2-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-29-8 CAPLUS

CN 2-Propanol, 1-[(2-furanylmethyl)amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-30-1 CAPLUS

CN 2-Propanol, 2-methyl-1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[[[4-(trifluoromethyl)phenyl]methyl]amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-31-2 CAPLUS

CN 2-Propanol, 2-methyl-1-[[(1R)-1-phenylethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

RN

330650-32-3 CAPLUS 2-Propanol, 2-methyl-1-[[(1S)-1-phenylethyl]amino]-3-(3-thieno[2,3-CNd]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

330650-33-4 CAPLUS 2-Propanol, 2-methyl-1-[(1-naphthalenylmethyl)amino]-3-(3-thieno[2,3-CNd]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-34-5 CAPLUS

2-Propanol, 2-methyl-1-[(4-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME) CN

RN 330650-35-6 CAPLUS

2-Propanol, 2-methyl-1-[(3-pyridinylmethyl)amino]-3-(3-thieno[2,3-CN d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

330650-36-7 CAPLUS 2-Propanol, 2-methyl-1-[(2-pyridinylmethyl)amino]-3-(3-thieno[2,3-CN d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

330650-37-8 CAPLUS RN

2-Propanol, 1-[(2-furanylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-CN ylphenoxy) -, monohydrochloride, (2R) - (9CI) (CA INDEX NAME)

#### ● HCl

RN 330650-38-9 CAPLUS

CN 2-Propanol, 1-[(3-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, dihydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

### ●2 HCl

RN 330650-39-0 CAPLUS

CN Benzenemethanol, α-[[(2R)-2-hydroxy-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]amino]methyl]-, monohydrochloride (9CI) (CAINDEX NAME)

Absolute stereochemistry.

### ● HCl

RN 330650-51-6 CAPLUS

CN Benzenemethanamine, N-[(2R)-2-methoxy-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### HCl

RN 330650-52-7 CAPLUS

CN Benzenemethanamine, N-[(2R)-2-methoxy-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-53-8 CAPLUS

CN Benzenemethanamine, N-[(2R)-2-methoxy-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# ● HCl

RN 330650-56-1 CAPLUS

CN 2-Propanol, 1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

RN 330650-57-2 CAPLUS

CN 2-Propanol, 1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2R)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 330650-56-1 CMF C19 H18 N2 O3 S2

Absolute stereochemistry.

CM 2

CRN 87-69-4 CMF C4 H6 O6

Absolute stereochemistry.

RN 330650-59-4 CAPLUS

CN 2-Propanol, 1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(3-thienylmethyl)amino]-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

### ● HCl

RN 330650-60-7 CAPLUS CN 2-Propanol, 1-[(1-naphthalenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

## ● HCl

RN 330650-61-8 CAPLUS
CN 2-Propanol, 1-[(1-naphthalenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-67-4 CAPLUS
CN 2-Propanol, 2-methyl-1-[(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-68-5 CAPLUS

CN 2-Propanol, 2-methyl-1-[(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 330650-67-4 CMF C22 H22 N2 O3 S

Absolute stereochemistry.

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 330650-69-6 CAPLUS

CN 2-Propanol, 2-methyl-1-[(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN

330650-70-9 CAPLUS 2-Propanol, 2-methyl-1-[(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX CNNAME)

- CM

330650-69-6 CMF C22 H22 N2 O3 S

Absolute stereochemistry. Rotation (-).

CM2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 330650-71-0 CAPLUS

2-Propanol, 2-methyl-1-[methyl(phenylmethyl)amino]-3-(3-thieno[2,3-CN d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

### ● HCl

RN 330650-72-1 CAPLUS

CN 2-Propanol, 1-[[(4-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-73-2 CAPLUS

CN 2-Propanol, 1-[[(2-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-74-3 CAPLUS

CN 2-Propanol, 1-[[(3-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

RN 330650-75-4 CAPLUS

CN 2-Propanol, 1-[[(4-chlorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-76-5 CAPLUS

CN 2-Propanol, 1-[[(2-chlorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-77-6 CAPLUS

CN 2-Propanol, 1-[[(3,4-dichlorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

RN 330650-78-7 CAPLUS

CN 2-Propanol, 2-methyl-1-[[(1R)-1-phenylethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-79-8 CAPLUS

CN 2-Propanol, 2-methyl-1-[[(1S)-1-phenylethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-82-3 CAPLUS

CN 2-Propanol, 2-methyl-1-[(1-naphthalenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-83-4 CAPLUS

CN 2-Propanol, 2-methyl-1-[[(4-methylphenyl)methyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

RN 330650-84-5 CAPLUS

CN 2-Propanol, 1-[[(4-methoxyphenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-85-6 CAPLUS

CN 2-Propanol, 1-[[(2-methoxyphenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-86-7 CAPLUS

CN 2-Propanol, 1-[(2-furanylmethyl)amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-87-8 CAPLUS

CN 2-Propanol, 2-methyl-1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-88-9 CAPLUS

CN 2-Propanol, 2-methyl-1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(3-thienylmethyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-89-0 CAPLUS

CN 2-Propanol, 2-methyl-1-[(3-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-90-3 CAPLUS

CN 2-Propanol, 2-methyl-1-[(2-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

330650-91-4 CAPLUS RN

2-Propanol, 2-methyl-1-[methyl(phenylmethyl)amino]-3-(3-thieno[2,3-CNd]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

330650-96-9 CAPLUS 2-Propanol, 1-[(1H-benzimidazol-2-ylmethyl)amino]-3-(3-thieno[2,3d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-98-1 CAPLUS

2-Propanol, 1-[(4-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

RN330650-99-2 CAPLUS CN 2-Propanol, 1-[(1,2,3,4-tetrahydro-1-naphthalenyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330651-04-2 CAPLUS

CN 2-Propanol, 1-[(2,3-dihydro-1H-inden-2-yl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 330651-05-3 CAPLUS

CN 2-Propanol, 1-[(2,3-dihydro-1H-inden-2-yl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330651-06-4 CAPLUS

CN 2-Propanol, 1-[(cyclohexylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

RN 330651-07-5 CAPLUS

CN 2-Propanol, 1-[(2,3-dihydro-1H-inden-1-yl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330651-08-6 CAPLUS

CN 2-Propanol, 1-[[(4-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 330651-09-7 CAPLUS

CN 2-Propanol, 1-[[(3,4-dichlorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

● HCl

RN

330651-10-0 CAPLUS 2-Propanol, 1-[[(3,4-difluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-CNd]isoxazol-3-ylphenoxy)-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HC1

330651-11-1 CAPLUS RN

2-Propanol, 1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-CN(tricyclo[3.3.1.13,7]dec-1-ylamino)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN330651-18-8 CAPLUS

2-Propanol, 1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(3-CN thienylmethyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

RN330651-21-3 CAPLUS

Benzenemethanol,  $\alpha$ -[[[(2R)-2-hydroxy-3-(3-thieno[2,3-d]isoxazol-3-CNylphenoxy)propyl]amino]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN330651-22-4 CAPLUS

CNBenzenemethanamine, N-[(2R)-2-methoxy-3-(3-thieno[2,3-d]isoxazol-3ylphenoxy)propyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN

330651-23-5 CAPLUS 2-Propanol, 1-[[(3,4-difluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-CN d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

RN 330672-14-5 CAPLUS

2-Propanol, 1-[methyl(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-CN ylphenoxy) -, (2R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

330651-36-0P IT

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 1-amino-3-thienoisoxazolylphenoxy-2-propanols as dopamine D4 antagonists)

330651-36-0 CAPLUS RN

2-Propanol, 1-[(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-CN ylphenoxy) -, (2R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

2

ACCESSION NUMBER:

2001:208281 CAPLUS

DOCUMENT NUMBER:

134:252333

TITLE:

Preparation of N-(aralkyl) (thienoisoxazolylphenoxy)alk

anamines and analogs as dopamine D4 antagonists Lee, George Ed; Ayers, Timothy A.; Jurcak, John G.

Aventis Pharmaceuticals, Inc., USA PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 108 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

INVENTOR(S):

English

1

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.				KINI	KIND DATE				APPLICATION NO.						DATE			
						-									-	<del>-</del>		
WO	2001	0198	32		<b>A</b> 2		2001	0322 1004		WO 2	000-1	US24:	949		2	0000	913	
WO	2001019832			<b>A</b> 3		2001	1004											
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              HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
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         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
              CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     EP 1216249
                            A2
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                                                EP 2000-964967
                                                                          20000913
     EP 1216249
                            B1
                                   20031119
              AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL
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                                                BR 2000-14513
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                                   20030415
                                                EE 2002-133
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                            Α
     AT 254620
                            Е
                                   20031215
                                                AT 2000-964967
                                                                          20000913
     PT 1216249
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                                   20030602
                                                ZA 2002-1760
     ZA 2002001760
                            Α
                                                                          20020301
     NO 2002001249
                                                NO 2002-1249
                                   20020510
                                                                          20020313
PRIORITY APPLN. INFO.:
                                                US 1999-396156
                                                                       A1 19990914
                                                WO 2000-US24949
                                                                          20000913
OTHER SOURCE(S):
                           MARPAT 134:252333
     ROZR3 [R3 = thieno[2,3-d]isoxazol-3-yl throughout][I; R = Z1NR1R2 or
     1-benzyl-3-pyrrolidinyl; R1 = CH2R4, CH2CH(OH)R4, CHMeR4, indanyl, etc.;
     R2 = H or alkyl; NR1R2 = heterocyclyl; R4 = cyclohexenyl, (hetero)aryl,
     etc.; Z = phenylene; Z1 = alkylene] were prepared Thus, 3-bromothiophene
     was acylated by 3-(MeO)C6H4COCl and the oximated product cyclized to give,
     after O-demethylation, 3-R3C6H4OH which was etherified by
     3-FC6H4CH2NHCOCH2Cl (preparation given) and the product reduced to give
     3-R3C6H4OCH2CH2NHCH2C6H4F-3. Data for biol. activity of I were given.
IT
     330678-80-3P 330678-81-4P 330678-82-5P
     330678-83-6P 330678-84-7P 330678-85-8P
     330678-86-9P 330678-87-0P 330678-88-1P
     330678-89-2P 330678-94-9P 330678-95-0P
     330679-25-9P 330679-26-0P 330679-27-1P
     330679-28-2P 330679-29-3P 330679-30-6P
     330679-33-9P 330679-35-1P 330679-36-2P
     330679-37-3P 330679-38-4P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
         (preparation of N-(aralkyl) (thienoisoxazolylphenoxy) alkanamines and analogs
        as dopamine D4 antagonists)
     330678-80-3 CAPLUS
RN
     Benzenemethanamine, 3-fluoro-N-[3-(3-thieno[2,3-d]isoxazol-3-
CN
     ylphenoxy)propyl] - (9CI) (CA INDEX NAME)
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RN 330678-81-4 CAPLUS
CN Benzenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-,
monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 330678-82-5 CAPLUS

CN Benzenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-(9CI) (CA INDEX NAME)

RN 330678-83-6 CAPLUS

CN Benzenemethanamine, 4-fluoro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330678-84-7 CAPLUS

CN Benzenemethanamine, 4-chloro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330678-85-8 CAPLUS

CN Benzenemethanamine, 4-methoxy-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330678-86-9 CAPLUS

CN 2-Thiophenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl](9CI) (CA INDEX NAME)

RN 330678-87-0 CAPLUS

CN 3-Thiophenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl](9CI) (CA INDEX NAME)

RN 330678-88-1 CAPLUS

CN 3-Pyridinemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl](9CI) (CA INDEX NAME)

RN 330678-89-2 CAPLUS

CN Benzenemethanol,  $\alpha$ -[[[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 330678-94-9 CAPLUS

CN Benzenesulfonamide, 4-[[[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 330678-95-0 CAPLUS

CN Benzenesulfonamide, 4-[2-[[3-(3-thieno[2,3-d]isoxazol-3-

ylphenoxy)propyl]amino]ethyl] - (9CI) (CA INDEX NAME)

RN 330679-25-9 CAPLUS

CN Benzenemethanamine, 4-methyl-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-26-0 CAPLUS

CN Benzenemethanamine, 2-chloro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-27-1 CAPLUS

CN Benzenemethanamine, 3-methoxy-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-28-2 CAPLUS

CN Benzenemethanamine, 3,4-difluoro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-29-3 CAPLUS

CN 1H-Inden-1-amine, 2,3-dihydro-N-[3-(3-thieno[2,3-d]isoxazol-3-

ylphenoxy)propyl] - (9CI) (CA INDEX NAME)

RN 330679-30-6 CAPLUS

CN 1H-Inden-2-amine, 2,3-dihydro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-33-9 CAPLUS

CN Tricyclo[3.3.1.13,7]decan-1-amine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-35-1 CAPLUS

CN Benzenemethanamine, 2,4-difluoro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-36-2 CAPLUS

CN Benzenemethanamine, 2,6-difluoro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

CN

RN330679-37-3 CAPLUS

> Benzenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-2-(trifluoromethyl) - (9CI) (CA INDEX NAME)

RN 330679-38-4 CAPLUS

Benzenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-4-CN (trifluoromethyl) - (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN 1987:598314 CAPLUS

ACCESSION NUMBER:

DOCUMENT NUMBER:

107:198314

TITLE:

Preparation of [(3-aminopropoxy)phenyl]thienoisoxazole s and-pyrazoles for treatment of hypertension and

glaucoma

INVENTOR(S): PATENT ASSIGNEE(S): Ong, Helen Hu; Yasenchak, Christine Mary Hoechst-Roussel Pharmaceuticals, Inc., USA

SOURCE:

Eur. Pat. Appl., 73 pp. CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
EP 221414	A1	19 <u>870</u> 513	EP 1986-114314	19861016		
R: AT, BE, CH	, DE, ES	, FR, GB,	GR, IT, LI, LU, NL, SE			
US 4728651	Α	19880301	US 1985-791019	19851024		
DK 8605079	Α	19870425	DK 1986-5079	19861023		
AU 8664337	A1	19870430	AU 1986-64337	19861023		
JP 62103086	A2	19870513	JP 1986-250937	19861023		
ZA 8608065	Α	19870624	ZA 1986-8065	19861023		
HU 45061	A2	19880530	HU 1986-4456	19861023		
HU 198058	В	19890728				
US 4769472	A	19880906	US 1987-125108	19871125		

10088250.trn

PRIORITY APPLN. INFO.:

US 1985-791019

19851024

OTHER SOURCE(S): GΙ

CASREACT 107:198314

The title compds. [I; X = O, NR; R = H, alkyl; R1 = H; R2 = alkyl, AΒ arylalkyl, aryloxyalkyl, indolylalkyl, benzodioxarylalkyl, or NR1R2 = (arylalkyl)piperazinyl] were prepared as antihypertensives and for reduction of intraocular pressure. 3-[(2-Epoxymethoxy)phenyl]-1-methyl-1H-thieno[3,2c]pyrazole 3 g was refluxed with Me3CNH2 in EtOH for 5 h to give 2.5 g of [(aminopropoxy)phenyl]thienopyrazole derivative (II).2HCl. II reduced outflow pressure by 51% when administered to an eye as a 2% solution

IT 110894-42-3P 110894-43-4P 110894-44-5P 110894-45-6P 110894-46-7P 110894-47-8P 110894-48-9P 110894-49-0P 110894-50-3P 110894-51-4P 110894-52-5P 110894-53-6P 110894-54-7P 110894-55-8P 110894-58-1P 110894-59-2P 110894-60-5P 110894-61-6P 110894-62-7P 110894-63-8P 110894-64-9P 110894-65-0P 110894-66-1P 110894-67-2P 110894-68-3P 110894-69-4P 110894-70-7P 110894-71-8P 110894-72-9P 110894-73-0P 110894-74-1P 110894-75-2P 110894-76-3P 110894-77-4P 110916-52-4P RL: SPN (Synthetic preparation); PREP (Preparation)

Ι

(preparation of, for treatment of hypertension and glaucoma)

RN110894-42-3 CAPLUS

2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-(2-thieno[2,3-d]isoxazol-3-CN ylphenoxy) - (9CI) (CA INDEX NAME)

110894-43-4 CAPLUS RN

2-Propanol, 1-[(1-methylethyl)amino]-3-(2-thieno[2,3-d]isoxazol-3-CNvlphenoxy) - (9CI) (CA INDEX NAME)

RN 110894-44-5 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-45-6 CAPLUS

CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-46-7 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-47-8 CAPLUS

CN 2-Propanol, 1-[(1-methyl-3-phenylpropyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-48-9 CAPLUS

CN 2-Propanol, 1-[(1-methyl-2-phenoxyethyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-49-0 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-43-4 CMF C17 H20 N2 O3 S

$$\begin{array}{c|c} & & & \\ & & & \\ i\text{-PrNH-CH}_2\text{-CH-CH}_2\text{-O} \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ \end{array}$$

CM 2

CRN 110-16-7 CMF C4 H4 O4 Double bond geometry as shown.

CN

RN 110894-50-3 CAPLUS

2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM I

CRN 110894-42-3 CMF C18 H22 N2 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-51-4 CAPLUS

CN 2-Propanol, 1-[(1-methyl-3-phenylpropyl)amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-52-5 CAPLUS

CN 2-Propanol, 1-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]amino]-3-(2-

Page 39

10/21/2004

10088250.trn

thieno[2,3-d]isoxazol-3-ylphenoxy)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 110894-53-6 CAPLUS

CN 2-Propanol, 1-[[2-(1H-indol-3-yl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

RN 110894-54-7 CAPLUS .

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, dihydrochloride (9CI) (CA INDEX NAME)

# ●2 HCl

RN 110894-55-8 CAPLUS
CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, dihydrochloride (9CI) (CA INDEX NAME)

# •2 HCl

CM 1

CRN 110894-47-8 CMF C25 H29 N3 O2 S

CM2

CRN 144-62-7 CMF C2 H2 O4

RN

110894-59-2 CAPLUS 2-Propanol, 1-[(1-methylethyl)amino]-3-(3-thieno[2,3-b]isoxazol-3-CNylphenoxy) - (9CI) (CA INDEX NAME)

RN

110894-60-5 CAPLUS 2-Propanol, 1-[(1-methylethyl)amino]-3-(3-thieno[2,3-b]isoxazol-3-ylphenoxy)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME) CN

CM1

CRN 110894-59-2 CMF C17 H20 N2 O3 S

CM2

CRN 110-16-7 CMF C4 H4 O4 Double bond geometry as shown.

RN 110894-61-6 CAPLUS

CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-(3-thieno[2,3-d]isoxazol-4-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-62-7 CAPLUS

CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-(3-thieno[2,3-d]isoxazol-4-ylphenoxy)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-61-6 CMF C18 H22 N2 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-63-8 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

# ● HCl

RN 110894-64-9 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-65-0 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-64-9 CMF C17 H20 N2 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-66-1 CAPLUS

CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-67-2 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

MeO 
$$CH_2-CH_2-NH-CH_2-CH-CH_2-O$$
 OH

RN 110894-68-3 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-67-2 CMF C24 H27 N3 O4 S

$$\begin{array}{c|c} \text{OMe} & & & \text{H} \\ \text{N} & & \text{N} \\ \text{S} & & & \text{N} \\ \text{CH}_2-\text{CH}_2-\text{NH}-\text{CH}_2-\text{CH}-\text{CH}_2-\text{O} \\ & & \text{OH} \\ \end{array}$$

CM 2

10088250.trn

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-69-4 CAPLUS

CN 2-Propanol, 1-[(1-methyl-2-phenoxyethyl)amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-70-7 CAPLUS

CN 2-Propanol, 1-[(1-methyl-2-phenoxyethyl)amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-69-4 CMF C23 H25 N3 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

10088250.trn

RN 110894-71-8 CAPLUS

CN 2-Propanol, 1-[[2-(2-methoxyphenoxy)ethyl]amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-72-9 CAPLUS

CN 2-Propanol, 1-[[2-(2-methoxyphenoxy)ethyl]amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, (2E)-2-butenedioate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-71-8 CMF C24 H27 N3 O4 S

$$\begin{array}{c|c} & \text{Me} \\ & \\ & \\ \text{N} \\ \\ \text{N} \\ \\ \text{O-CH}_2-\text{CH}_2-\text{NH-CH}_2-\text{CH-CH}_2-\text{O} \\ \\ & \\ \text{OH} \\ \end{array}$$

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-73-0 CAPLUS

CN 2-Propanol, 1-[[2-(2-methoxyphenoxy)-1-methylethyl]amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-74-1 CAPLUS

2-Propanol, 1-[[2-(2-methoxyphenoxy)-1-methylethyl]amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CN

CRN 110894-73-0 CMF C25 H29 N3 O4 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-75-2 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-[3-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN

110894-76-3 CAPLUS 2-Propanol, 1-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME) CN

RN110894-77-4 CAPLUS

2-Propanol, 1-[(1-methylethyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-CNc]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \\ & \\ \text{N} \\ \\ \text{I-PrNH-CH}_2-\text{CH-CH}_2-\text{O} \\ \\ \\ \text{OH} \\ \end{array}$$

RN110916-52-4 CAPLUS

CN 2-Propanol, 1-[[2-(1H-indol-3-yl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3ylphenoxy) - (9CI) (CA INDEX NAME)

=> FIL REGISTRY
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 19.56 175.19

FULL ESTIMATED COST

· SINCE FILE TOTAL

CA SUBSCRIBER PRICE

ENTRY SESSION -2.10 -2.10

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STRUCTURE FILE UPDATES: 20 OCT 2004 HIGHEST RN 766487-31-4 DICTIONARY FILE UPDATES: 20 OCT 2004 HIGHEST RN 766487-31-4

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

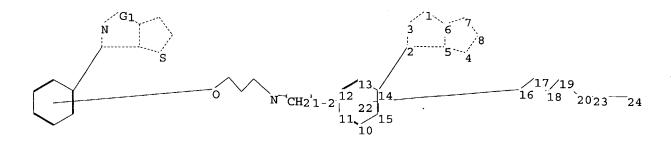
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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> Uploading C:\Program Files\Stnexp\Queries\10088250a.str



chain nodes : 16 17 18 19 20 23 24 ring nodes : 1 2 3 4 5 6 7 8 10 11 12 13 14 15 chain bonds : 2-14 16-17 17-18 18-19 19-20 20-23 23-24 ring bonds : 1-6 1-3 2-5 2-3 4-5 4-8 5-6 6-7 7-8 10-11 10-15 11-12 12-13 13-14 14-15 exact/norm bonds : 1-6 1-3 2-5 2-3 2-14 4-5 4-8 5-6 6-7 7-8 16-17 17-18 18-19 19-20 20-23 23-24 normalized bonds :  $10 - 11 \quad 10 - 15 \quad 11 - 12 \quad 12 - 13 \quad 13 - 14 \quad 14 - 15$ isolated ring systems : containing 1 : 10 :

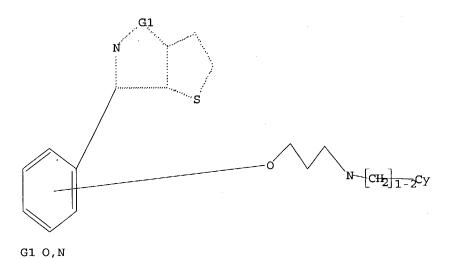
### G1:0,N

#### Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 23:CLASS 24:Atom

# L5 \_, STRUCTURE UPLOADED

=> d 15 L5 HAS NO ANSWERS L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15

SAMPLE SEARCH INITIATED 09:02:38 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 5 TO ITERATE

3 ANSWERS 100.0% PROCESSED 5 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

5 TO 234 PROJECTED ITERATIONS:

PROJECTED ANSWERS: 3 TO 163

3 SEA SSS SAM L5 1.6

=> s 15 sss full

FULL SEARCH INITIATED 09:02:45 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 134 TO ITERATE

100.0% PROCESSED 134 ITERATIONS 89 ANSWERS

SEARCH TIME: 00.00.01

89 SEA SSS FUL L5

=> FIL CAPLUS

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 157.94 333.13

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

-2.10 CA SUBSCRIBER PRICE 0.00

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FILE COVERS 1907 - 21 Oct 2004 VOL 141 ISS 17 FILE LAST UPDATED: 20 Oct 2004 (20041020/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L8
             3 L7
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L3
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1.4
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1.5
L6
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L8 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:208282 CAPLUS

DOCUMENT NUMBER: 134:237472

TITLE: Preparation of 1-amino-3-thienoisoxazolylphenoxy-2-

propanols as dopamine D4 antagonists

10/21/2004

10088250.trn

INVENTOR(S): Fink, David M.; Freed, Brian S.; Hrib, Nicholas J.; Kosley, Raymond W., Jr.; Lee, George E.; Merriman,

Gregory H.; Rauckman, Barbara S. Aventis Pharmaceuticals, Inc., USA

PATENT ASSIGNEE(S): SOURCE:

PCT Int. Appl., 157 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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WO	2001019833					A1 20010322			WO 2000-US24962									
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OTHER SOURCE(S): MARPAT 134:237472

AB RZOCH2CR1R2CH2NR3R4 [I; R = e.g., thieno[2,3-d]isoxazol-3-yl; R1 = OH or alkoxy; R2,R4 = H or alkyl; R3 = CH2R5, CH2CH(OH)R5, indanyl, etc.; R5 = cyclohex(en)yl, (hetero)aryl, etc.; Z = phenylene] were prepared Thus, 3-bromothiophene was acylated by 3-(MeO)C6H4COCl and the oximated product cyclized to give, after O-demethylation, 3-RC6H4OH [R = thieno[2,3-d]isoxazol-3-yl] which was etherified by (R)-glycidyl tosylate and the product aminated by PhCHMeNH2 to give (R)-3-RC6H4OCH2CH(OH)CH2NMeCH2Ph (R as above). Data for biol. activity of I were given.

RN CN

Absolute stereochemistry. Rotation (+).

#### ● HCl

RN 330650-17-4 CAPLUS
CN 2-Propanol, 1-[(2-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-18-5 CAPLUS

CN 2-Propanol, 1-[(1-naphthalenylmethyl)amino]-3-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

RN 330650-19-6 CAPLUS

CN 2-Propanol, 1-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(3-thienylmethyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-20-9 CAPLUS

CN 2-Propanol, 1-[(2-furanylmethyl)amino]-3-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-21-0 CAPLUS

CN 2-Propanol, 1-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

RN 330650-22-1 CAPLUS

CN 2-Propanol, 2-methyl-1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-23-2 CAPLUS

CN 2-Propanol, 2-methyl-1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2R)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 330650-22-1 CMF C20 H20 N2 O3 S2

Absolute stereochemistry.

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 330650-24-3 CAPLUS

CN 2-Propanol, 1-[[(4-methoxyphenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-25-4 CAPLUS

CN 2-Propanol, 1-[[(2-methoxyphenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-26-5 CAPLUS

CN 2-Propanol, 1-[[(4-chlorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-27-6 CAPLUS

CN 2-Propanol, 1-[[(4-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

RN

330650-28-7 CAPLUS 2-Propanol, 1-[[(2-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-CN dlisoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

330650-29-8 CAPLUS RN

2-Propanol, 1-[(2-furanylmethyl)amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-CN3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-30-1 CAPLUS

2-Propanol, 2-methyl-1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[[[4-CN(trifluoromethyl)phenyl]methyl]amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN330650-33-4 CAPLUS CN 2-Propanol, 2-methyl-1-[(1-naphthalenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-34-5 CAPLUS

CN 2-Propanol, 2-methyl-1-[(4-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-35-6 CAPLUS

CN 2-Propanol, 2-methyl-1-[(3-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-36-7 CAPLUS

CN 2-Propanol, 2-methyl-1-[(2-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

RN 330650-37-8 CAPLUS

CN 2-Propanol, 1-[(2-furanylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# ● HCl

RN 330650-38-9 CAPLUS

CN 2-Propanol, 1-[(3-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, dihydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# ●2 HC1

RN 330650-51-6 CAPLUS

CN Benzenemethanamine, N-[(2R)-2-methoxy-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 330650-52-7 CAPLUS

CN Benzenemethanamine, N-[(2R)-2-methoxy-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-53-8 CAPLUS

CN Benzenemethanamine, N-[(2R)-2-methoxy-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HC1

RN 330650-56-1 CAPLUS

CN 2-Propanol, 1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

RN

330650-57-2 CAPLUS 2-Propanol, 1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-CNthienylmethyl)amino]-, (2R)-, (2R,3R)-2,3-dihydroxybutanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM1

CRN 330650-56-1 CMF C19 H18 N2 O3 S2

Absolute stereochemistry.

CM2

CRN 87-69-4 C4 H6 O6 CMF

Absolute stereochemistry.

RN330650-59-4 CAPLUS

CN2-Propanol, 1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(3thienylmethyl)amino]-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

## ● HCl

RN 330650-60-7 CAPLUS

CN 2-Propanol, 1-[(1-naphthalenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

# ● HCl

RN 330650-61-8 CAPLUS

CN 2-Propanol, 1-[(1-naphthalenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-67-4 CAPLUS

CN 2-Propanol, 2-methyl-1-[(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-68-5 CAPLUS

CN 2-Propanol, 2-methyl-1-[(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 330650-67-4 CMF C22 H22 N2 O3 S

Absolute stereochemistry.

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 330650-69-6 CAPLUS

CN 2-Propanol, 2-methyl-1-[(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 330650-70-9 CAPLUS

CN 2-Propanol, 2-methyl-1-[(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 330650-69-6 CMF C22 H22 N2 O3 S

Absolute stereochemistry. Rotation (-).

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 330650-71-0 CAPLUS

CN 2-Propanol, 2-methyl-1-[methyl(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2R)- (9CI) (CA INDEX NAME)

#### ● HCl

RN 330650-72-1 CAPLUS
CN 2-Propanol, 1-[[(4-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-73-2 CAPLUS

CN 2-Propanol, 1-[[(2-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-74-3 CAPLUS

CN 2-Propanol, 1-[[(3-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

RN

330650-75-4 CAPLUS 2-Propanol, 1-[[(4-chlorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-CN d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

330650-76-5 CAPLUS RN

2-Propanol, 1-[[(2-chlorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-CN d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-77-6 CAPLUS

CN2-Propanol, 1-[[(3,4-dichlorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3dlisoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

RN 330650-82-3 CAPLUS

CN 2-Propanol, 2-methyl-1-[(1-naphthalenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-83-4 CAPLUS

CN 2-Propanol, 2-methyl-1-[[(4-methylphenyl)methyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-84-5 CAPLUS

CN 2-Propanol, 1-[[(4-methoxyphenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-85-6 CAPLUS

CN 2-Propanol, 1-[[(2-methoxyphenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

RN 330650-86-7 CAPLUS

CN 2-Propanol, 1-[(2-furanylmethyl)amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-87-8 CAPLUS

CN 2-Propanol, 2-methyl-1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(2-thienylmethyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-88-9 CAPLUS

CN 2-Propanol, 2-methyl-1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(3-thienylmethyl)amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-89-0 CAPLUS

CN 2-Propanol, 2-methyl-1-[(3-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-90-3 CAPLUS

CN 2-Propanol, 2-methyl-1-[(2-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-91-4 CAPLUS

CN 2-Propanol, 2-methyl-1-[methyl(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330650-96-9 CAPLUS

CN 2-Propanol, 1-[(1H-benzimidazol-2-ylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

RN 330650-98-1 CAPLUS

CN 2-Propanol, 1-[(4-pyridinylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330651-06-4 CAPLUS

CN 2-Propanol, 1-[(cyclohexylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330651-08-6 CAPLUS

CN 2-Propanol, 1-[[(4-fluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

● HCl

RN 330651-09-7 CAPLUS

CN 2-Propanol, 1-[[(3,4-dichlorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 330651-10-0 CAPLUS

CN 2-Propanol, 1-[[(3,4-difluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 330651-18-8 CAPLUS

Page 73

CN 2-Propanol, 1-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-3-[(3-thienylmethyl)amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330651-22-4 CAPLUS

CN Benzenemethanamine, N-[(2R)-2-methoxy-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330651-23-5 CAPLUS

CN 2-Propanol, 1-[[(3,4-difluorophenyl)methyl]amino]-2-methyl-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 330672-14-5 CAPLUS

CN 2-Propanol, 1-[methyl(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

330651-36-0P IT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 1-amino-3-thienoisoxazolylphenoxy-2-propanols as dopamine D4 antagonists)

330651-36-0 CAPLUS RN

2-Propanol, 1-[(phenylmethyl)amino]-3-(3-thieno[2,3-d]isoxazol-3-CN ylphenoxy) -, (2R) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVALLABLE IN THE RE FORMAT

Preparation of N (aralkyl) (thienoisoxazolylphenoxy) alk

anamines and analogs as dopamine D4 antagonists Lee, George E Ayers, Timothy A.; Jurcak, John G.

L8ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

2

ACCESSION NUMBER:

2001:208281 CAPLUS 134:252333

DOCUMENT NUMBER:

TITLE:

INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

LANGUAGE:

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT:

English 1

PATENT INFORMATION:

Patent

CODEN: PIXXD2

PATENT NO.	KIND DATE	E APPLICAT	ION NO.	DATE
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WO 2001019832	A2 2001	.0322 WO 2000-	US24949	20000913
WO 2001019832	A3 2001	.1004		
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CR, CU, C	Z, DE, DK, DM,	DZ, EE, ES, FI,	GB, GD, GE,	GH, GM, HR,
HU, ID, I	L, IN, IS, JP,	KE, KG, KP, KR,	KZ, LC, LK,	LR, LS, LT,
LU, LV, M	A, MD, MG, MK,	MN, MW, MX, MZ,	NO, NZ, PL,	PT, RO, RU,
SD, SE, S	G, SI, SK, SL,	TJ, TM, TR, TT,	TZ, UA, UG,	US, UZ, VN,
YU, ZA, Z	W, AM, AZ, BY,	KG, KZ, MD, RU,	TJ, TM	
RW: GH, GM, K	E, LS, MW, MZ,	SD, SL, SZ, TZ,	UG, ZW, AT,	BE, CH, CY,

Aventis Pharmaceuticals, Inc., USA PCT Int. Appl., 108 pp.

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             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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                                20031119
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PRIORITY APPLN. INFO.:
                                             US 1999-396156
                                                                 A1 19990914
                                             WO 2000-US24949
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OTHER SOURCE(S):
                         MARPAT 134:252333
     ROZR3 [R3 = thieno[2,3-d]isoxazol-3-yl throughout][I; R = Z1NR1R2 or
     1-benzyl-3-pyrrolidinyl; R1 = CH2R4, CH2CH(OH)R4, CHMeR4, indanyl, etc.;
     R2 = H or alkyl; NR1R2 = heterocyclyl; R4 = cyclohexenyl, (hetero)aryl,
     etc.; Z = phenylene; Z1 = alkylene] were prepared Thus, 3-bromothiophene
     was acylated by 3-(MeO)C6H4COCl and the oximated product cyclized to give,
     after O-demethylation, 3-R3C6H4OH which was etherified by
     3-FC6H4CH2NHCOCH2Cl (preparation given) and the product reduced to give
     3-R3C6H4OCH2CH2NHCH2C6H4F-3. Data for biol. activity of I were given.
     330678-80-3P 330678-81-4P 330678-82-5P
TT
     330678-83-6P 330678-84-7P 330678-85-8P
     330678-86-9P 330678-87-0P 330678-88-1P
     330678-94-9P 330678-95-0P 330679-25-9P
     330679-26-0P 330679-27-1P 330679-28-2P
     330679-35-1P 330679-36-2P 330679-37-3P
     330679-38-4P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of N-(aralkyl) (thienoisoxazolylphenoxy) alkanamines and analogs
        as dopamine D4 antagonists)
RN
     330678-80-3 CAPLUS
     Benzenemethanamine, 3-fluoro-N-[3-(3-thieno[2,3-d]isoxazol-3-
CN
     ylphenoxy)propyl] - (9CI) (CA INDEX NAME)
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RN 330678-81-4 CAPLUS
CN Benzenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-,
monohydrochloride (9CI) (CA INDEX NAME)

#### ● HCl

RN 330678-82-5 CAPLUS

CN Benzenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl](9CI) (CA INDEX NAME)

RN 330678-83-6 CAPLUS

CN Benzenemethanamine, 4-fluoro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330678-84-7 CAPLUS

CN Benzenemethanamine, 4-chloro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330678-85-8 CAPLUS

CN Benzenemethanamine, 4-methoxy-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330678-86-9 CAPLUS

CN 2-Thiophenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-(9CI) (CA INDEX NAME)

RN 330678-87-0 CAPLUS

CN 3-Thiophenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-(9CI) (CA INDEX NAME)

RN 330678-88-1 CAPLUS

CN 3-Pyridinemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl](9CI) (CA INDEX NAME)

RN 330678-94-9 CAPLUS

CN Benzenesulfonamide, 4-[[[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 330678-95-0 CAPLUS

CN Benzenesulfonamide, 4-[2-[[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 330679-25-9 CAPLUS

CN Benzenemethanamine, 4-methyl-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-26-0 CAPLUS

CN Benzenemethanamine, 2-chloro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-27-1 CAPLUS

CN Benzenemethanamine, 3-methoxy-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-28-2 CAPLUS

CN Benzenemethanamine, 3,4-difluoro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN 330679-35-1 CAPLUS

CN Benzenemethanamine, 2,4-difluoro-N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]- (9CI) (CA INDEX NAME)

RN330679-36-2 CAPLUS

CNBenzenemethanamine, 2,6-difluoro-N-[3-(3-thieno[2,3-d]isoxazol-3ylphenoxy)propyl] - (9CI) (CA INDEX NAME)

RN330679-37-3 CAPLUS

Benzenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-2-CN (trifluoromethyl) - (9CI) (CA INDEX NAME)

RN330679-38-4 CAPLUS

Benzenemethanamine, N-[3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)propyl]-4-CN(trifluoromethyl) - (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1987:598314 CAPLUS

DOCUMENT NUMBER:

107:198314

TITLE:

Preparation of [(3-aminopropoxy)phenyl]thienoisoxazole

s and- pyrazoles for treatment of hypertension and

glaucoma

INVENTOR(S):

Ong, Helen Hu; Yasenchak, Christine Mary

PATENT ASSIGNEE(S):

Hoechst-Roussel Pharmaceuticals, Inc., USA

SOURCE:

Eur. Pat. Appl., 73 pp. CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

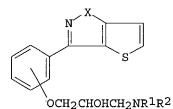
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PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 221414	A1	19870513	EP 1986-114314	19861016
R: AT, BE, CH,	DE, ES	, FR, GB, (	GR, IT, LI, LU, NL, SE	
US 4728651	A	19880301	US 1985-791019	19851024
DK 8605079	A	19870425	DK 1986-5079	19861023
AU 8664337	'A1	19870430	AU 1986-64337	19861023
DK 8605079	A	19870425	DK 1986-5079	19861023

#### 10088250.trn

#### 10/21/2004

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ZA	8608065	Α	19870624	ZA	1986-8065	1	9861023
HU	45061	A2	19880530	HU	1986-4456	. 1	9861023
HU	198058	В	19890728				
US	4769472	Α	19880906	US	1987-125108	1	9871125
PRIORITY	APPLN. INFO.:			US	1985-791019	1	9851024
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GI							



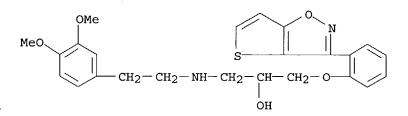
AB The title compds. [I; X = O, NR; R = H, alkyl; R1 = H; R2 = alkyl, arylalkyl, aryloxyalkyl, indolylalkyl, benzodioxarylalkyl, or NR1R2 = (arylalkyl)piperazinyl] were prepared as antihypertensives and for reduction of intraocular pressure. 3-[(2-Epoxymethoxy)phenyl]-1-methyl-1H-thieno[3,2-c]pyrazole 3 g was refluxed with Me3CNH2 in EtOH for 5 h to give 2.5 g of [(aminopropoxy)phenyl]thienopyrazole derivative (II).2HCl. II reduced outflow pressure by 51% when administered to an eye as a 2% solution

IT 110894-44-5P 110894-46-7P 110894-52-5P 110894-53-6P 110894-63-8P 110894-67-2P 110894-68-3P 110894-76-3P 110916-52-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for treatment of hypertension and glaucoma)

RN 110894-44-5 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)



RN 110894-46-7 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-52-5 CAPLUS

CN 2-Propanol, 1-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 110894-53-6 CAPLUS

CN 2-Propanol, 1-[[2-(1H-indol-3-yl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

RN 110894-63-8 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

HC1

RN 110894-67-2 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OMe} \\ \text{MeO} \\ \\ \text{CH}_2-\text{CH}_2-\text{NH}-\text{CH}_2-\text{CH}-\text{CH}_2-\text{O} \\ \\ \text{OH} \\ \end{array}$$

RN 110894-68-3 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-67-2 CMF C24 H27 N3 O4 S

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-76-3 CAPLUS

CN 2-Propanol, 1-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110916-52-4 CAPLUS

CN 2-Propanol, 1-[[2-(1H-indol-3-yl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

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L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

PATENT ASSIGNEE(S):

1987:598314 CAPLUS

DOCUMENT NUMBER:

107:198314

TITLE:

Preparation of [(3-aminopropoxy)phenyl]thienoisoxazole

s and- pyrazoles for treatment of hypertension and

glaucoma

INVENTOR(S):

Ong, Helen Hu; Yasenchak, Christine Mary Hoechst-Roussel Pharmaceuticals, Inc., USA

SOURCE:

Eur. Pat. Appl., 73 pp.

CODEN: EPXXDW

DOCUMENT TYPE: LANGUAGE: Patent English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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HU 198058	B 1989072	28	
US 4769472	A 1988090	06 US 1987-125108	19871125 <
PRIORITY APPLN. INFO.:		US 1985-791019	19851024
OTHER SOURCE(S):	CASREACT 107:1	198314	

GΙ

Me

The title compds. [I; X = Q, NR; R = H, alkyl; R1 = H; R2 = alkyl, arylalkyl, aryloxyalkyl, indolylalkyl, benzodioxarylalkyl, or NR1R2 = (arylalkyl)piperazinyl] were prepared as antihypertensives and for reduction of intraocular pressure. 3-[(2-Epoxymethoxy)phenyl]-1-methyl-1H-thieno[3,2-c]pyrazole 3 g was refluxed with Me3CNH2 in EtOH for 5 h to give 2.5 g of [(aminopropoxy)phenyl]thienopyrazole derivative (II).2HCl. II reduced outflow pressure by 51% when administered to an eye as a 2% solution

IT 110894-42-3P 110894-43-4P 110894-44-5P 110894-45-6P 110894-46-7P 110894-47-8P 110894-48-9P 110894-49-0P 110894-50-3P 110894-51-4P 110894-52-5P 110894-53-6P 110894-59-2P 110894-55-8P 110894-58-1P 110894-62-7P 110894-63-8P 110894-64-9P 110894-65-0P 110894-66-1P 110894-67-2P 110894-68-3P 110894-72-9P 110894-71-8P 110894-72-9P 110894-73-0P

110894-71-8P 110894-72-9P 110894-73-0P 110894-74-1P 110894-75-2P 110894-76-3P

110894-77-4P 110916-52-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, for treatment of hypertension and glaucoma)

RN 110894-42-3 CAPLUS

CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-43-4 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ i - PrNH - CH_2 - CH - CH_2 - O \\ & & & \\ OH \end{array}$$

RN 110894-44-5 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} & & & \\ \text{MeO} & & & \\ \text{S} & & & \\ \text{CH}_2-\text{CH}_2-\text{NH}-\text{CH}_2-\text{CH}-\text{CH}_2-\text{O} \\ \\ \text{OH} & & \\ \end{array}$$

RN 110894-45-6 CAPLUS

CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-46-7 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-47-8 CAPLUS

CN 2-Propanol, 1-[(1-methyl-3-phenylpropyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-48-9 CAPLUS

CN 2-Propanol, 1-[(1-methyl-2-phenoxyethyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-49-0 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-43-4 CMF C17 H20 N2 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

$$HO_2C$$
 Z  $CO_2H$ 

RN

110894-50-3 CAPLUS 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-(2-thieno[2,3-d]isoxazol-3-CNylphenoxy) -, (2Z) -2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM

110894-42-3 C18 H22 N2 O3 S CMF

CM2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

110894-51-4 CAPLUS RN

CN 2-Propanol, 1-[(1-methyl-3-phenylpropyl)amino]-3-(2-thieno[2,3-d]isoxazol3-ylphenoxy) - (9CI) (CA INDEX NAME)

RN 110894-52-5 CAPLUS

CN 2-Propanol, 1-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

#### ● HCl

RN 110894-53-6 CAPLUS

CN 2-Propanol, 1-[[2-(1H-indol-3-yl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

RN 110894-54-7 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-

c]pyrazol-3-yl)phenoxy]-, dihydrochloride (9CI) (CA INDEX NAME)

## ●2 HC1

RN 110894-55-8 CAPLUS
CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, dihydrochloride (9CI) (CA INDEX NAME)

# ●2 HCl

RN 110894-58-1 CAPLUS
CN 2-Propanol, 1-[(1-methyl-3-phenylpropyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, ethanedioate (1:1) (salt) (9CI) (CAINDEX NAME)

CM 1

CRN 110894-47-8 CMF C25 H29 N3 O2 S

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 110894-59-2 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-(3-thieno[2,3-b]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-60-5 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-(3-thieno[2,3-b]isoxazol-3-ylphenoxy)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-59-2 CMF C17 H20 N2 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4 Double bond geometry as shown.

RN 110894-61-6 CAPLUS

CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-(3-thieno[2,3-d]isoxazol-4-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-62-7 CAPLUS

CN 2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-(3-thieno[2,3-d]isoxazol-4-ylphenoxy)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-61-6 CMF C18 H22 N2 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-63-8 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

## ● HCl

RN 110894-64-9 CAPLUS
CN 2-Propanol, 1-[(1-methylethyl)amino]-3-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-65-0 CAPLUS CN 2-Propanol, 1-[(1-methylethyl)amino]-3-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-64-9 CMF C17 H20 N2 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

CN

RN 110894-66-1 CAPLUS

2-Propanol, 1-[(1,1-dimethylethyl)amino]-3-(4-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-67-2 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} & & & \text{H} \\ \text{N} & & \text{N} \\ \text{S} & & & \text{N} \\ \text{CH}_2-\text{CH}_2-\text{NH}-\text{CH}_2-\text{CH}-\text{CH}_2-\text{O} \\ \text{OH} & & \text{OH} \\ \end{array}$$

RN 110894-68-3 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-67-2 CMF C24 H27 N3 O4 S

MeO 
$$\begin{array}{c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

CM 2

10088250.trn

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-69-4 CAPLUS

CN 2-Propanol, 1-[(1-methyl-2-phenoxyethyl)amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-70-7 CAPLUS

CN 2-Propanol, 1-[(1-methyl-2-phenoxyethyl)amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-69-4 CMF C23 H25 N3 O3 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

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RN 110894-71-8 CAPLUS

CN 2-Propanol, 1-[[2-(2-methoxyphenoxy)ethyl]amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

OMe S 
$$\sim$$
 OH  $\sim$  
RN 110894-72-9 CAPLUS

CN 2-Propanol, 1-[[2-(2-methoxyphenoxy)ethyl]amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, (2E)-2-butenedioate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-71-8 CMF C24 H27 N3 O4 S

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-73-0 CAPLUS

CN 2-Propanol, 1-[[2-(2-methoxyphenoxy)-1-methylethyl]amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-74-1 CAPLUS

CN 2-Propanol, 1-[[2-(2-methoxyphenoxy)-1-methylethyl]amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, (2Z)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-73-0 CMF C25 H29 N3 O4 S

CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-75-2 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-[3-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

RN 110894-76-3 CAPLUS

CN 2-Propanol, 1-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-77-4 CAPLUS

CN 2-Propanol, 1-[(1-methylethyl)amino]-3-[2-(1-methyl-1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \\ & \\ \text{i-PrNH-CH}_2-\text{CH-CH}_2-\text{O} \\ & \\ & \\ \text{OH} \end{array}$$

RN 110916-52-4 CAPLUS

CN 2-Propanol, 1-[[2-(1H-indol-3-yl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

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L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:

1987:598314 CAPLUS

DOCUMENT NUMBER:

107:198314

TITLE:

Preparation of [(3-aminopropoxy)phenyl]thienoisoxazole

s and- pyrazoles for treatment of hypertension and

glaucoma

INVENTOR(S):

PATENT ASSIGNEE(S):

Ong, Helen Hu; Yasenchak, Christine Mary Hoechst-Roussel Pharmaceuticals, Inc., USA

SOURCE:

Eur. Pat. Appl., 73 pp. CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
EP 221414	A1 19870513	EP 1986-114314	19861016 <
R: AT, BE, CH,	DE, ES, FR, GB,	GR, IT, LI, LU, NL, SE	•
US 4728651	A 19880301	US 1985-791019	19851024 <
DK 8605079	A 19870425	DK 1986-5079	19861023 <
AU 8664337	A1 19870430	AU 1986-64337	19861023 <
JP 62103086	A2 19870513	JP 1986-250937	19861023 <
ZA 8608065	A 19870624	ZA 1986-8065	19861023 <
HU 45061	A2 19880530	HU 1986-4456	19861023 <
HU 198058	B 19890728		
US 4769472	A 19880906	US 1987-125108	19871125 <
PRIORITY APPLN. INFO.:		US 1985-791019	19851024
OTHER SOURCE(S):	CASREACT 107:198	314	
CT			

GI

AB The title compds. [I; X = O, NR; R = H, alkyl; R1 = H; R2 = alkyl, arylalkyl, aryloxyalkyl, indolylalkyl, benzodioxarylalkyl, or NR1R2 = (arylalkyl)piperazinyl] were prepared as antihypertensives and for reduction of intraocular pressure. 3-[(2-Epoxymethoxy)phenyl]-1-methyl-1H-thieno[3,2-c]pyrazole 3 g was refluxed with Me3CNH2 in EtOH for 5 h to give 2.5 g of [(aminopropoxy)phenyl]thienopyrazole derivative (II).2HCl. II reduced outflow pressure by 51% when administered to an eye as a 2% solution

IT 110894-44-5P 110894-46-7P 110894-52-5P 110894-53-6P 110894-63-8P 110894-67-2P 110894-68-3P 110894-76-3P 110916-52-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, for treatment of hypertension and glaucoma)

RN 110894-44-5 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-46-7 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

RN 110894-52-5 CAPLUS

CN 2-Propanol, 1-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 110894-53-6 CAPLUS

CN 2-Propanol, 1-[[2-(1H-indol-3-yl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

RN 110894-63-8 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-(3-thieno[2,3-d]isoxazol-3-ylphenoxy)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

## 10/21/2004

RN 110894-67-2 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]- (9CI) (CA INDEX NAME)

MeO 
$$CH_2-CH_2-NH-CH_2-CH-CH_2-O$$
 OH

RN 110894-68-3 CAPLUS

CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-[2-(1H-thieno[3,2-c]pyrazol-3-yl)phenoxy]-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 110894-67-2 CMF C24 H27 N3 O4 S

MeO 
$$CH_2-CH_2-NH-CH_2-CH-CH_2-O$$
 OH

CM 2

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.

RN 110894-76-3 CAPLUS

CN 2-Propanol, 1-[[(2,3-dihydro-1,4-benzodioxin-2-yl)methyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

10088250.trn

$$\begin{array}{c|c} O & & & & \\ \hline O & & & \\ \hline O & & \\ O & & \\ \hline O & \\ CH_2-NH-CH_2-CH-CH_2-O \\ \hline \\ OH \\ \end{array}$$

RN 110916-52-4 CAPLUS

CN 2-Propanol, 1-[[2-(1H-indol-3-yl)ethyl]amino]-3-(2-thieno[2,3-d]isoxazol-3-ylphenoxy)- (9CI) (CA INDEX NAME)

=> log y SINCE FILE TOTAL COST IN U.S. DOLLARS ENTRY SESSION 29.20 362.33 FULL ESTIMATED COST DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL **ENTRY** SESSION CA SUBSCRIBER PRICE -3.50 -5.60

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